Chem 442: Homework for lecture L29

(only turn in **BOLD** assignment first lecture next week of classes; do <u>all</u> assignments)

1. In class, we evaluated three terms in the Hartree-Fock energy expression. Evaluate the remaining terms in the energy expression for 2 electrons in the ground state, to show that

$$E_{HF} = h_1 + h_2 + J_{12} - K_{12}$$

   [Hint: You may need to prove things like $\langle 12|V_{12}|12\rangle = \langle 21|V_{12}|21\rangle$; what is the relation between $r_{12} = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$ and r_{21} ?]

2. **Turn in** Problem 7.1 in the book.

3. Problem 8.2 in the book.